

Nonanoic acid, tert-butyldimethylsilyl ester

Other names:	Nonanoic acid, DMTBS Nonanoic acid, TBDMS Pelargonic acid, DMTBS tert-Butyl(dimethyl)silyl nonanoate Nonanoic acid, tbdms derivative
Inchi:	InChI=1S/C15H32O2Si/c1-7-8-9-10-11-12-13-14(16)17-18(5,6)15(2,3)4/h7-13H2,1-6H3
InchiKey:	UFZLLJFNHSSVAN-UHFFFAOYSA-N
Formula:	C15H32O2Si
SMILES:	CCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	272.50
CAS:	104255-73-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.01		Crippen Method
logp	5.285		Crippen Method
rinpol	1588.20		NIST Webbook
rinpol	1578.00		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1588.20		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1585.00		NIST Webbook
ripol	1638.00		NIST Webbook
ripol	1638.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104255734&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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